

```
#R CMD INSTALL \\Aa.ad.epa.gov\ord\RTP\Users\E-J\jwambaug\NETMyD~1\Resear~1\LiverPBPK
```

```
#setwd("\\Aa\ord\RTP\USers\E-J\jwambaug\NET MyDocuments\Research Projects\LiverPBPK")
```

```
Make.Wetmore.Plot(Wetmore,ExpoCast,ylim=c(10^-12,10^4))
```

```
Make.Wetmore.Plot(Wetmore,ExpoCast,ylim=c(10^-12,10^3),CAS.end=37)
```

```
Make.Wetmore.Plot(Wetmore,ExpoCast,ylim=c(10^-12,10^3),CAS.start=38,CAS.end=74)
```

```
Make.Wetmore.Plot(Wetmore,Wetmore.Exposures,predictions.lower.col=NULL,predictions.mean.col="Exposure.Estimates..mg.kg.day.",predictions.CAS.col="CASRN",predictions.nearfield.col=NULL,ylim=c(10^-12,10^4))
```

```
Make.Wetmore.Plot(Wetmore,Wetmore.Exposures,predictions.lower.col=NULL,random.suppress=0.1,predictions.mean.col="Exposure.Estimates..mg.kg.day.",predictions.CAS.col="CASRN",predictions.nearfield.col=NULL,ylim=c(10^-12,10^4))
```

```
Make.Wetmore.Plot(Wetmore,predictions.lower.col=NULL,cex.compound=0.15,ylab="AC50 (uM)",dose.lower.col="AC50",dose.order.col="Lower.Oral.Equivalent.mg.kg.",predictions.mean.col="Exposure.Estimates..mg.kg.day.",predictions.CAS.col="CASRN",predictions.nearfield.col=NULL,ylim=c(10^-5,10^4))
```

```
Make.Wetmore.Plot(Wetmore,predictions.lower.col=NULL,cex.compound=0.15,predictions.mean.col="Exposure.Estimates..mg.kg.day.",predictions.CAS.col="CASRN",predictions.nearfield.col=NULL,ylim=c(10^-5,10^4))
```

```
Make.Wetmore.Plot(Wetmore,Wetmore.Exposures,predictions.lower.col=NULL,predictions.mean.col="Exposure.Estimates..mg.kg.day.",predictions.CAS.col="CASRN",predictions.nearfield.col=NULL,ylim=c(10^-12,10^4))
```

```
UVPKM <-
```

```
function(model,fixed.params,which.quantile=0.95,CV.params=NULL,unif.params=NULL,samples=1000)
```

```
{
  sample.vec <- rep(NA,samples)
  for (this.sample in 1:samples)
  {
    these.params <- fixed.params
    for (this.param in names(CV.params))
    {
      these.params[[this.param]] <-
rnorm(1,mean=CV.params[[this.param]]$mean,sd=CV.params[[this.param]]$mean*CV.params[[this.param]]$CV)
    }
    for (this.param in names(unif.params))
    {
      these.params[[this.param]] <-
runif(1,min=unif.params[[this.param]]$min,max=unif.params[[this.param]]$max)
    }
    sample.vec[this.sample] <- call(model,these.params)
  }

  return(quantile(sample.vec,which.quantile))
}
```

```
Calc_1comp_Css <- function(chem.name=NULL,chem.CAS=NULL,daily.dose=1,which.quantile=0.95)
```

```
{  
}
```

```
Wetmore_Css(chem.CAS="94-82-6")  
Wetmore_Css(chem.CAS="94-82-6",which.quantile=0.5)
```

```
calc_Css(chem.CAS="94-82-6")
```

```
Wetmore_Oral_Equiv(4,chem.CAS="94-82-6")  
Wetmore_Oral_Equiv(6,chem.CAS="94-82-6")  
Wetmore_Oral_Equiv(6,chem.CAS="94-82-6",species="Rat")  
Wetmore_Oral_Equiv(6,chem.CAS="94-75-7",species="Rat",which.quantile=0.5)
```

```
Wetmore.human.values <- NULL  
vLiver.human.values <- NULL  
for (this.CAS in get_Wetmore_CAS())  
  if (this.CAS %in% get_Css_CAS())  
  {  
    Wetmore.human.values[this.CAS] <- Wetmore_Css(chem.CAS=this.CAS,which.quantile=0.5)  
    vLiver.human.values[this.CAS] <- calc_Css(parameterize_SteadyState(this.CAS))  
  }
```

```
plot(vLiver.human.values,Wetmore.human.values,log="xy")  
matplot(c(10^-3,10^2),c(10^-3,10^2),lty=2,add=T,type="l")
```

```
these.params <- parameterize_SteadyState("94-82-6")  
vary.params <- list(BW=list(mean=70,CV=0.2))  
vary.params[["liver.volume.per.kgBW"]]<-list(mean=0.02448,CV=0.2)  
UVPKM("calc_Css",these.params)
```